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Nonlinear Problems and Numerical Methods in
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13. ABSTRACT (Maximum 200 words)

By extension from our previous work on so called Case II diffusion, models have been developed to account for several kinds of anomalous non-Fickian diffusion. We have applied them to various problems arising from the uses of certain modern polymeric materials in novel applications in pharmaceutical devices, separating membranes for controlled gaseous and liquid mixing, and methods of adhesive bonding. In addition to the formulation in which important parameter groupings were identified analytical, asymptotic, and numerical methods were modified or devised to study the problems.

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**Nonlinear Problems and Numerical Methods in
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Publications and summaries of work

Free boundary problems in controlled release pharmaceuticals.

I: Diffusion in glassy polymers.

SIAM J. Appl. Math., Vol.48, No.6, (1988).

Donald S. Cohen and Thomas Erneux

This paper formulates and studies two different problems occurring in the formation and use of pharmaceuticals via controlled release methods. These problems involve a glassy polymer and a penetrant, and the central problem is to predict and control the diffusive behavior of the penetrant through the polymer. The mathematical theory yields free boundary problems which are studied in various asymptotic regimes.

Free boundary problems in controlled release pharmaceuticals:

II Swelling-controlled release.

SIAM J. Appl. Math., Vol.48, No.6, (1988).

Donald S. Cohen and Thomas Erneux

A problem in controlled release pharmaceutical systems is formulated and studied. The device modeled is a polymer matrix containing an initially immobilized drug. The release of the drug is achieved by countercurrent diffusion through a penetrant solvent with the release rate being determined by the rate of diffusion of the solvent in the polymer. The mathematical theory yields a free boundary problem which is studied in various asymptotic regimes.

A mathematical model for stress-driven diffusion in polymers.

Journal of Polymer Science: Part B: Polymer Physics, Vol.27, 589-602 (1989).

Robert W. Cox and Donald S. Cohen

A model for case II diffusion into polymers is presented. The addition of stress terms to the Fickian flux is used to produce the characteristic progressive front. The stress in turn obeys a concentration-dependent evolution equation. The model equations are analyzed in the limit of small diffusivity for the problem of penetration into a semiinfinite medium. Provided that the coefficient functions obey two monotonicity conditions, the solvent concentration profile is shown to have a steep front that progresses into the medium. The formulas governing the progression of the front are developed. After the front decays away, the long time behavior of the solution is shown to be a similarity solution as in Fickian diffusion. Two techniques for approximating the solvent concentration and the front position are presented. The first approximation method is a series expansion; formulas are given for the initial speed and deceleration of the front. The second approximation method uses a portion of the long time similarity solution to represent the short time solution behind the front.

Sharp fronts due to diffusion and stress at the glass transition in polymers.

Journal of Polymer Science: Part B: Polymer Physics, Vol.27, 1931-1747 (1989).

Donald S. Cohen and Andrew B. White, Jr.

We derive and analyze a model for sharp fronts in glassy polymers. We take the major effect of a diffusing penetrant on the polymer entanglement network to be the inducement of a differential viscoelastic stress. This couples diffusive and mechanical processes through a viscoelastic response where the strain depends upon the amount of penetrant present. Analytically, the major effect is to produce explicit delay terms, via a relaxation parameter, to account for the fundamental difference between a polymer in its rubbery state and the polymer in its glassy state, namely the finite relaxation time in the glassy state owing to slow response to changing conditions. We produce concentration profiles in good agreement with observations on sharp front formation. In addition the model can account for the phenomenon of sorption overshoot.

Delayed diffusion due to flux limitation.

Physics Letters A, Vol.142, No.1, 26-30 (1989).

P. Rosenau, P.S. Hagan, R.L. Northcutt and D.S. Cohen.

Consider a flux-limited diffusion process, where $u_t = [G(u_x)]_x$ with $G(\infty) < \infty$ and $G'(s) \geq 0$. We show that if the profile $u(0, x)$ initially has a sharp front, then the sharp front may not be resolved immediately. Instead, the front may remain perfectly sharp for a finite time, during which the height of the jump decays to zero. In this case the profile near the sharp front takes a self-similar form $u = \sqrt{t} f(x/\sqrt{t})$, with the front remaining sharp for a time $[h/2f(0)]^2$, where h is the height of the initial discontinuity. We also determine when an initially sharp jump will remain sharp for a finite time, and when it will be resolved immediately.

Changing time history in moving boundary problems.

SIAM J. Appl. Math. Vol.50, No.2, 483-489 (1990).

Donald S. Cohen and Thomas Erneux

A class of diffusion-stress equations modeling transport of solvent in glassy polymers is considered. The problem is formulated as a one-phase Stefan problem. It is shown that the moving front changes like \sqrt{t} initially but quickly behaves like t as t increases. The t behavior is typical of stress-dominated transport. The quasi-steady state approximation is used to analyze the time history of the moving front. This analysis is motivated by the small time solution.

*Asymptotic methods for metal oxide semiconductor
field effect transistor modeling.*

SIAM J. Appl. Math. Vol.50, No.4, 1099-1125 (1990).

M.J. Ward, F.M. Odeh and D.S. Cohen

The behavior of metal oxide semiconductor field effect transistors (MOSFETs) with small aspect ratio and large doping levels is analyzed using formal perturbation techniques. Specifically, the influence of interface layers in the potential on the averaged channel conductivity is closely examined. The interface and internal layers that occur in the potential are resolved in the limit of large doping using the method of matched asymptotic expansions. This approach, together with other asymptotic techniques, provides both a pointwise description of the state variables as well as lumped current-voltage relations that vary uniformly across the various bias regimes. These current-voltage relations are derived for a variable doping model representing a particular class of devices.

Sharp fronts due to diffusion and viscoelastic relaxation in polymers.

SIAM J. Appl. Math. Vol.51, No.2, 472-483 (1991).

Donald S. Cohen and Andrew B. White, Jr.

A model for sharp fronts in glassy polymers is derived and analyzed. The major effect of a diffusing penetrant on the polymer entanglement network is taken to be the inducement of a differential viscoelastic stress. This couples diffusive and mechanical processes through a viscoelastic response where the strain depends upon the amount of penetrant present. Analytically, the major effect is to produce explicit delay terms via a relaxation parameter. This accounts for the fundamental difference between a polymer in its rubbery state and the polymer in its glassy state, namely the finite relaxation time in the glassy state due to slow response to changing conditions. Both numerical and analytical perturbation studies of a boundary value problem for a dry glass polymer exposed to penetrant solvent are completed. Concentration profiles in good agreement with observations are obtained.

The evolution of steep fronts in non-Fickian polymer-penetrant systems.

Journal of Polymer Science: part B: Polymer Physics, Vol.30, 145-161 (1992).

Catherine K. Hayes and Donald S. Cohen

We adapt a recently proposed model for non-Fickian diffusion of penetrants into polymers and use it to study a drug-delivery problem. The model modifies Fick's diffusion equation by the addition of stress-induced flux. A stress evolution equation incorporating aspects of the Maxwell and Kelvin-Voigt viscoelastic stress models completes the model. The relaxation time in the polymer is taken as a function of the penetrant concentration. The system is studied under the assumption that the diffusivity is large. Singular perturbation techniques are used to show that the concentration and stress evolve diffusively for small time, but exhibit steep fronts in a narrow region within the domain for larger time. These predictions are verified numerically for specified parameter values. Finally, the equations are studied in the steady state and are found to predict the evolution of shocks.

Ph.D. degrees awarded

1990

Hayes, Catherine Kent
Diffusion and Stress Driven Flow in Polymers
Advisor: D.S. Cohen

McLachlan, Robert
Separated Viscous Flows via Multigrid.
Advisor: H.B. Keller

1992

Lui, Shiu-Hong
I. *Multiple Bifurcations.*
II. *Parallel Homotopy Method for the Real Nonsymmetric Eigenvalue Problem.*
Advisor: H.B. Keller

Melman, Aharon
Complexity Analysis for the Newton Modified Barrier Function Method.
Advisor: H.B. Keller

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